Modeling Protein/Ligand Interactions in Water

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Interactions between proteins in aqueous solutions affect their biological functions and determine the stability of the solutions with respect to phase transformations. Questions abound regarding the role of small solution components in these protein interactions. While some argue that small ions merely screen electrostatic interactions between proteins, others favor the view that the ions play a more active role and change protein solvent structures, thus altering the protein intermolecular interactions. We model the interaction between protein fragments and small ions using a combined explicit and implicit approach to study the effect of small ions on protein properties.